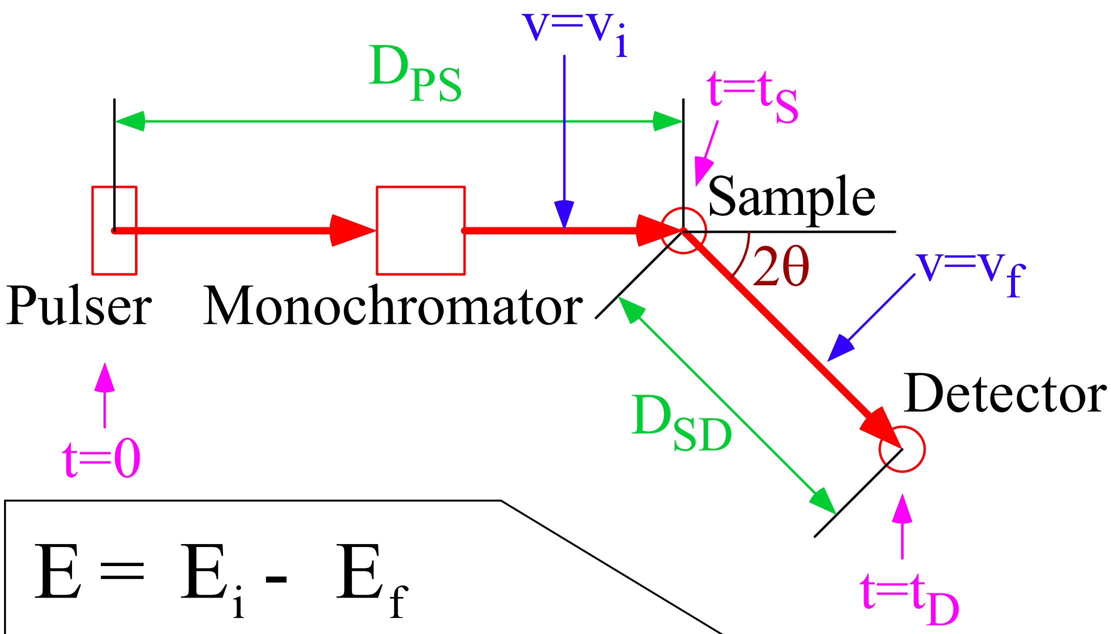
Time of flight (TOF) spectroscopy

How time of flight spectroscopy works

- in principle
- in practice (at the NCNR)

Trading intensity for resolution

TOF spectroscopy, *in principle*



$$E = E_i - E_f$$

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos(2q)$$

$$t_S = \frac{D_{PS}}{v_i}$$

$$v_f = \frac{D_{SD}}{t_D - t_S}$$

$$E_{i,f} = \frac{1}{2} m v_{i,f}^2$$

$$m v_{i,f} = h k_{i,f}$$

$$= \frac{h}{l_{i,f}}$$

Number of neutrons scattered at angle 2θ into solid angle $\Delta\Omega$, reaching detector within time interval $t_D, t_D+\Delta t$

(MEASURED)

Number of neutrons per unit area in incident beam

$$I(2\theta, t_D) = N\Phi \frac{d^2\sigma}{d\Omega dt} \Delta\Omega \Delta t$$

Number of atoms illuminated

Double differential scattering cross section (w.r.t. time)

Double differential scattering cross section (w.r.t. time)

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt}\frac{dt}{dE_f}$$

$$E_f = \tfrac{1}{2} m \left(\frac{D_{SD}}{t_{SD}}\right)^2$$

$$dE_f \propto \frac{1}{t_{SD}^3}\, dt$$

$$\therefore \frac{d^2\sigma}{d\Omega dE_f} \propto \frac{d^2\sigma}{d\Omega dt}\, t_{SD}^3$$

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_B}{4\pi\hbar}\frac{k_f}{k_i} S(Q,\omega)$$

$$k_f \propto \frac{1}{t_{SD}}$$

Hence $S(Q,\omega) \propto \frac{d^2\sigma}{d\Omega dt}\, t_{SD}^4$

Scattering function

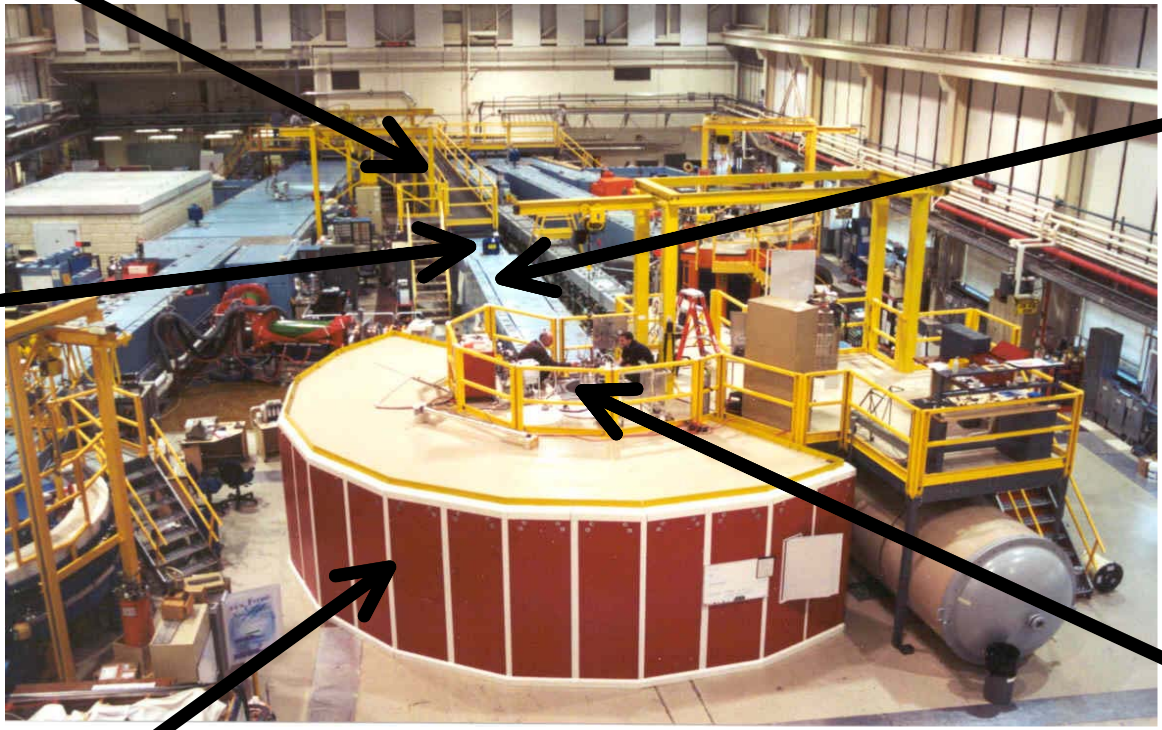
(DESIRED)

TOF spectroscopy, *in practice*

The NCNR Disk Chopper Spectrometer

(1) The neutron guide

(2) The crystal filter

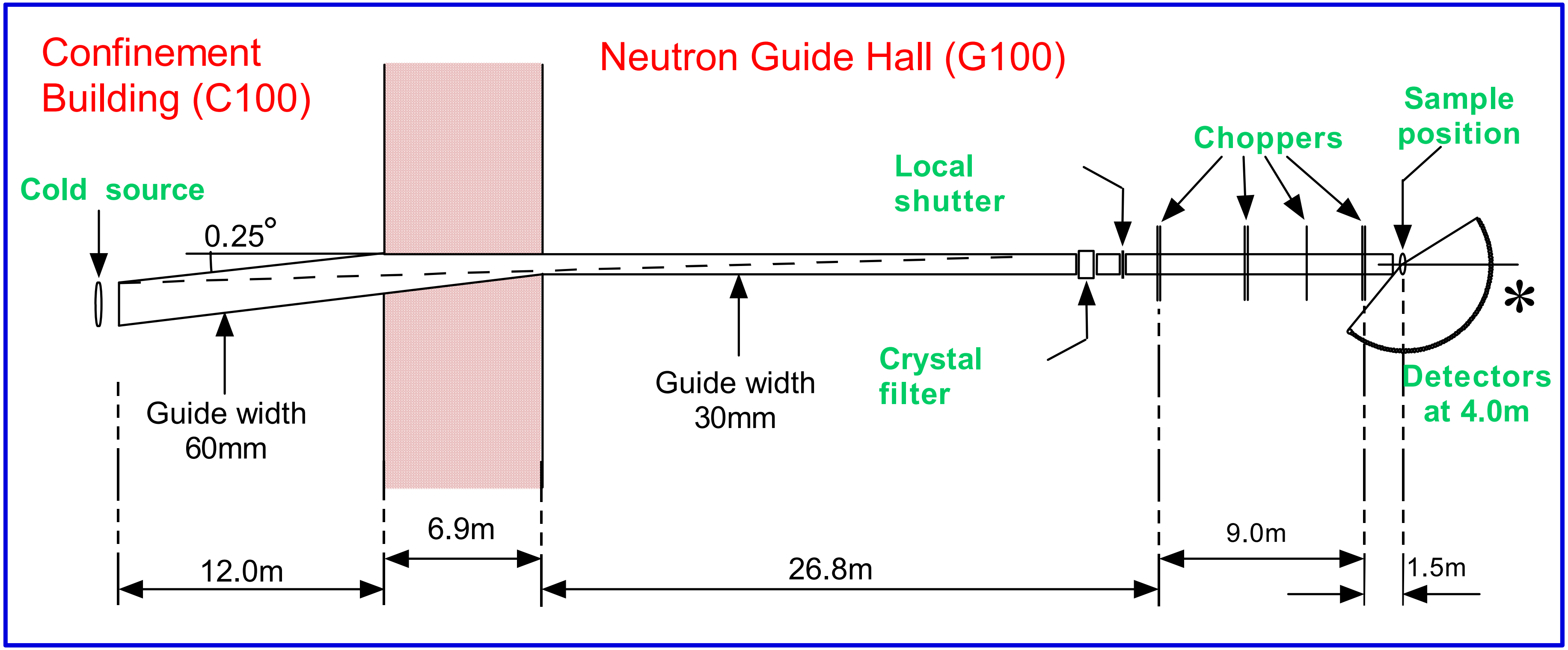


(3) The choppers

(4) The sample area

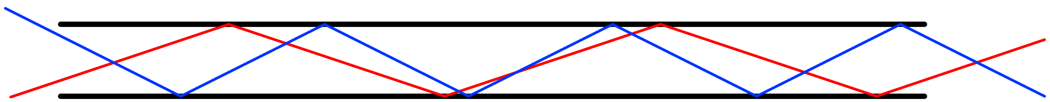
(5) The flight chamber and the detectors

Overall plan view of DCS (to scale)

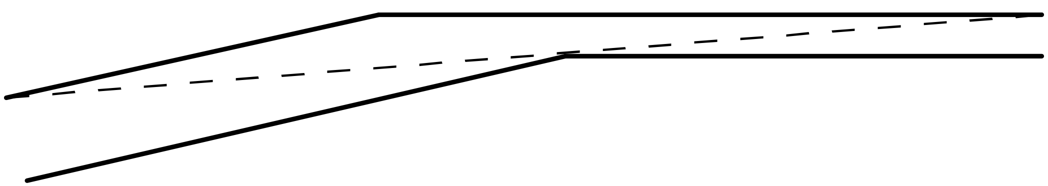


(1) The neutron guide

Neutrons transported by total external reflection; critical angle ✪wavelength.



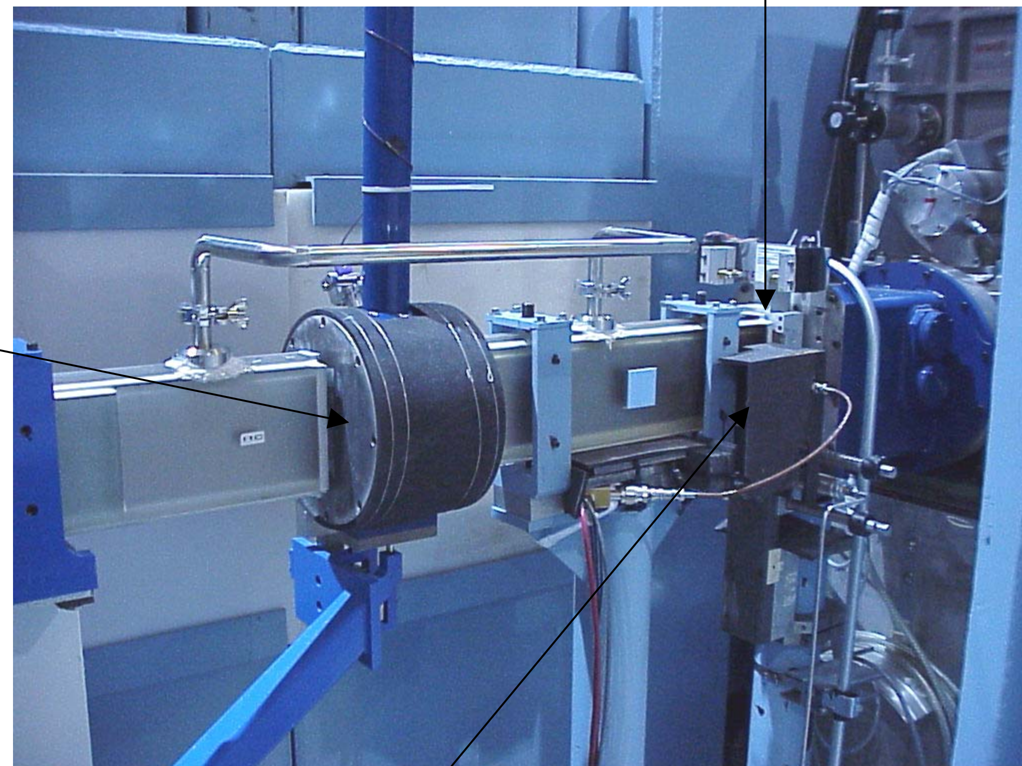
Gammas and high energy neutrons removed by "optical filter" design.



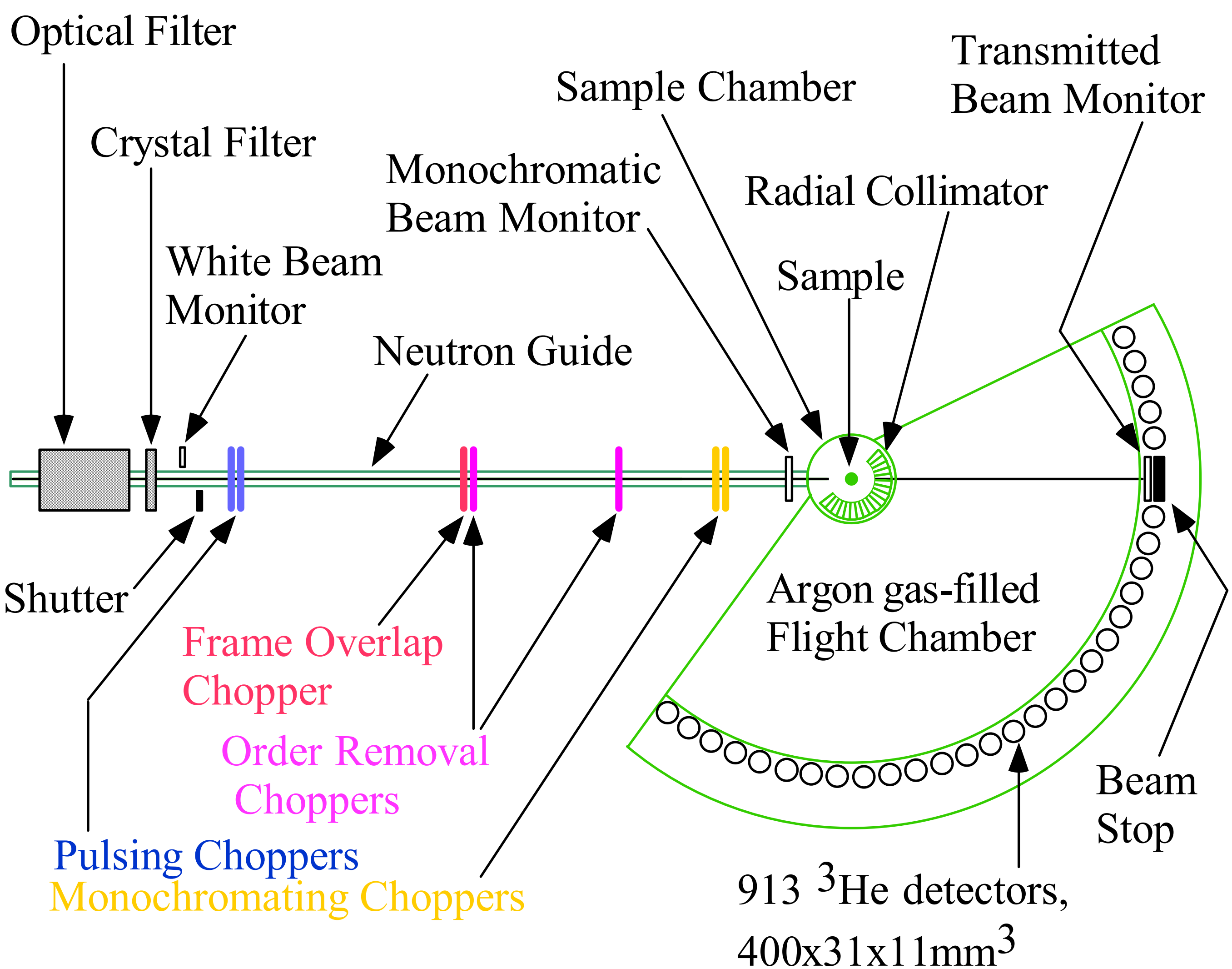
(2) The crystal filter

Shutter

Short wavelength neutrons removed by Bragg reflection in cooled pyrolytic graphite filter.



White beam monitor

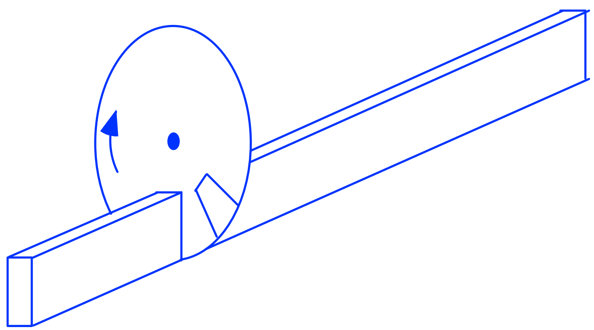


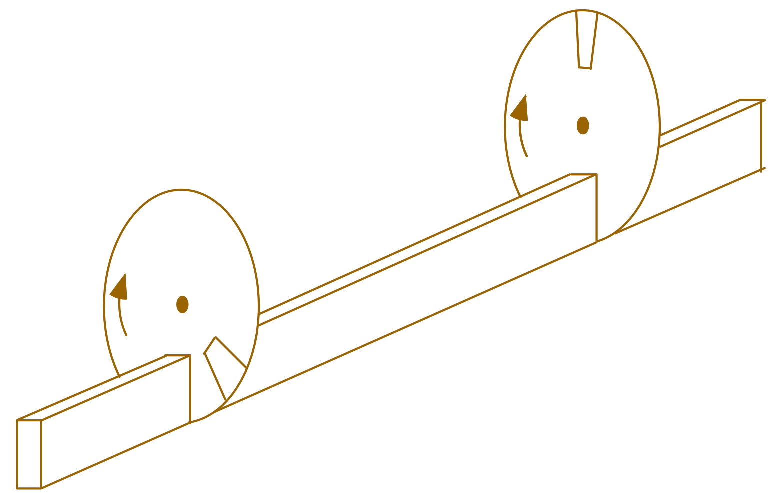
Optical Filter
Crystal Filter
White Beam Monitor
Neutron Guide
Monochromatic Beam Monitor
Sample Chamber
Transmitted Beam Monitor
Radial Collimator
Sample
Shutter
Frame Overlap Chopper
Order Removal Choppers
Pulsing Choppers
Monochromating Choppers
Argon gas-filled Flight Chamber
Beam Stop
913 ^{3}He detectors,
400x31x11mm^3

(3) The choppers

A single (disk) chopper pulses the neutron beam.

A second chopper selects neutrons within a narrow range of speeds.

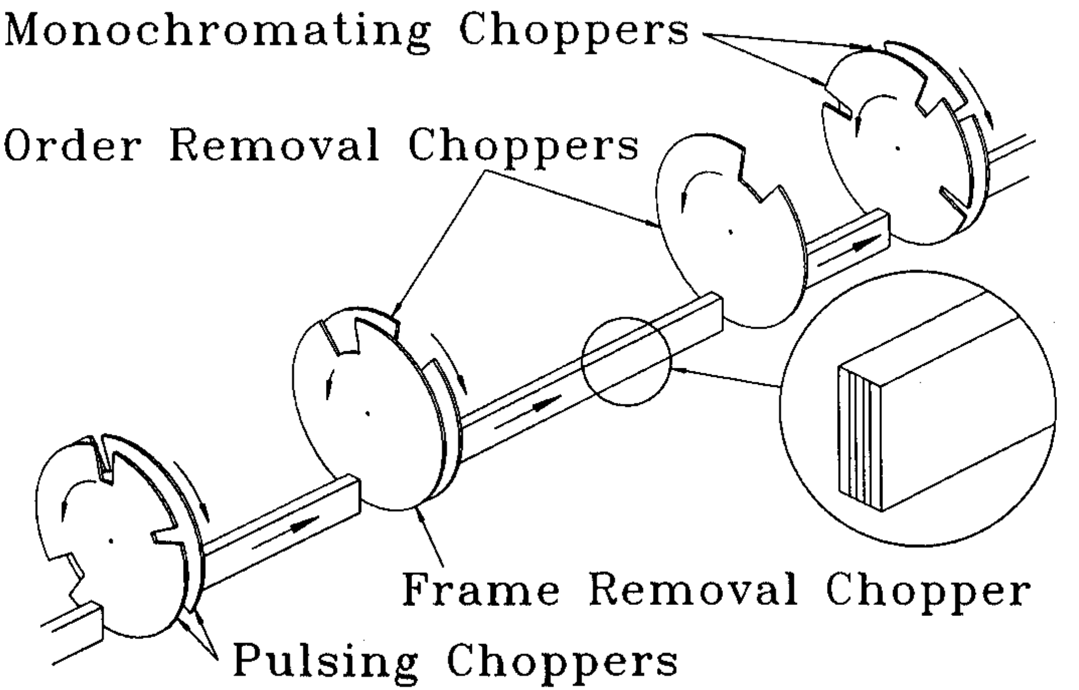




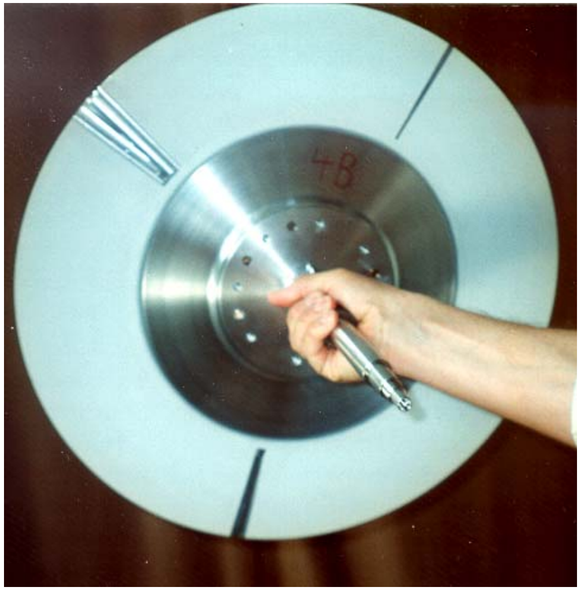
Counter-rotating choppers (close together), with speed ◆, behave like single choppers with speed 2◆. They can also permit a choice of pulse widths.

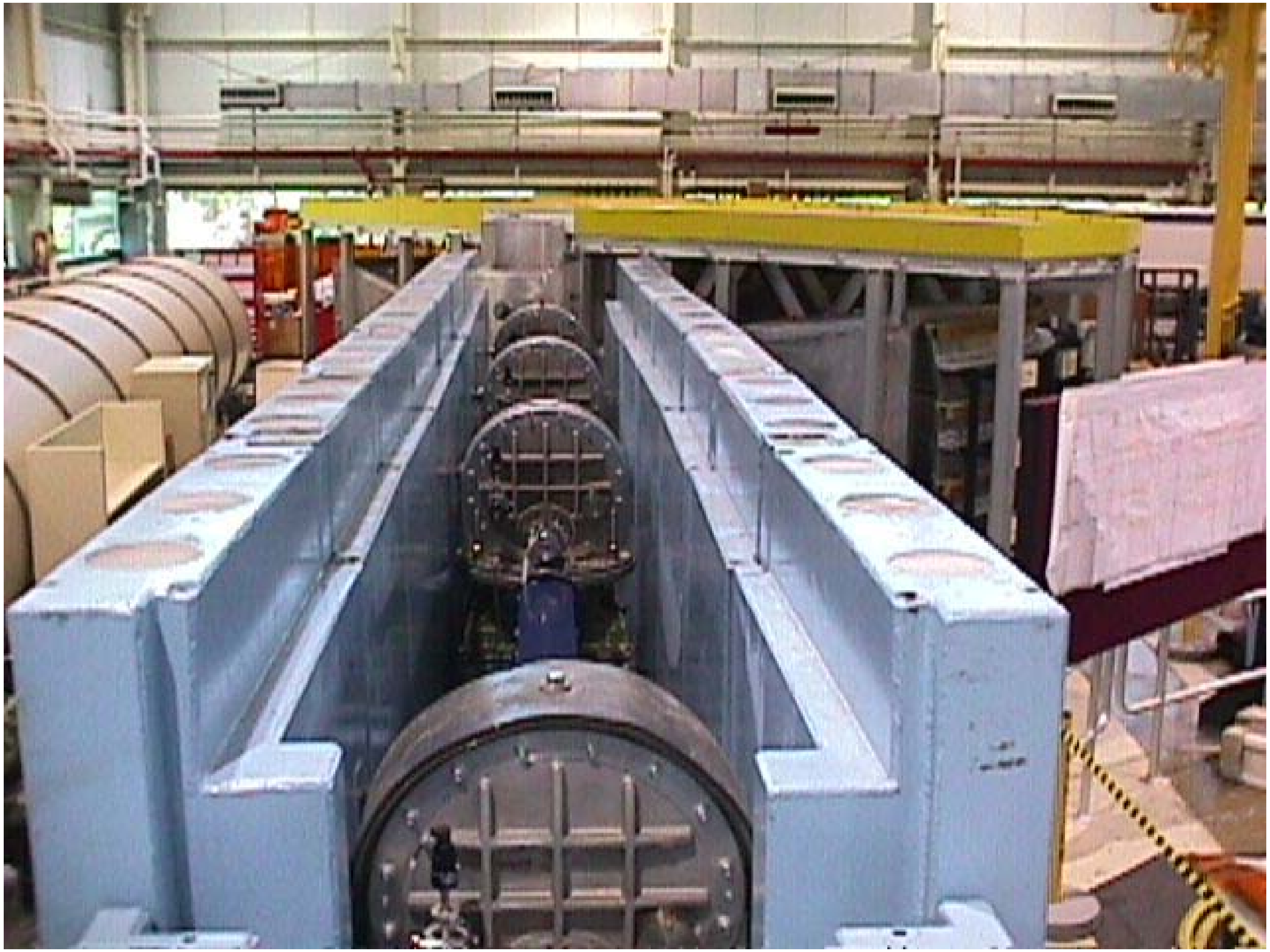
Additional choppers remove “contaminant” wavelengths and reduce the pulse frequency at the sample position.

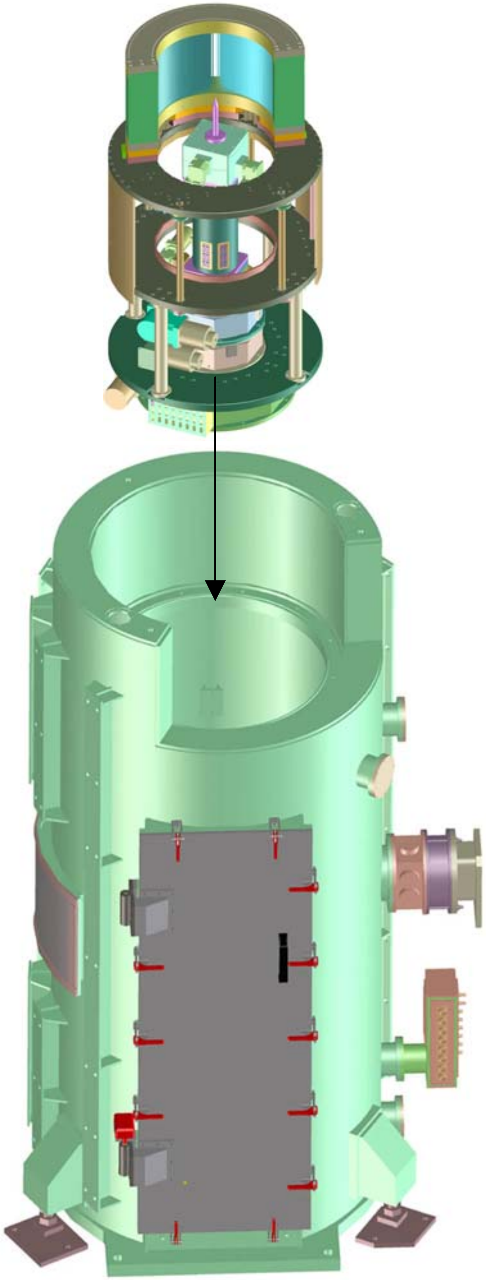
The DCS has seven choppers, 4 of which have 3 “slots”



Disk 4B

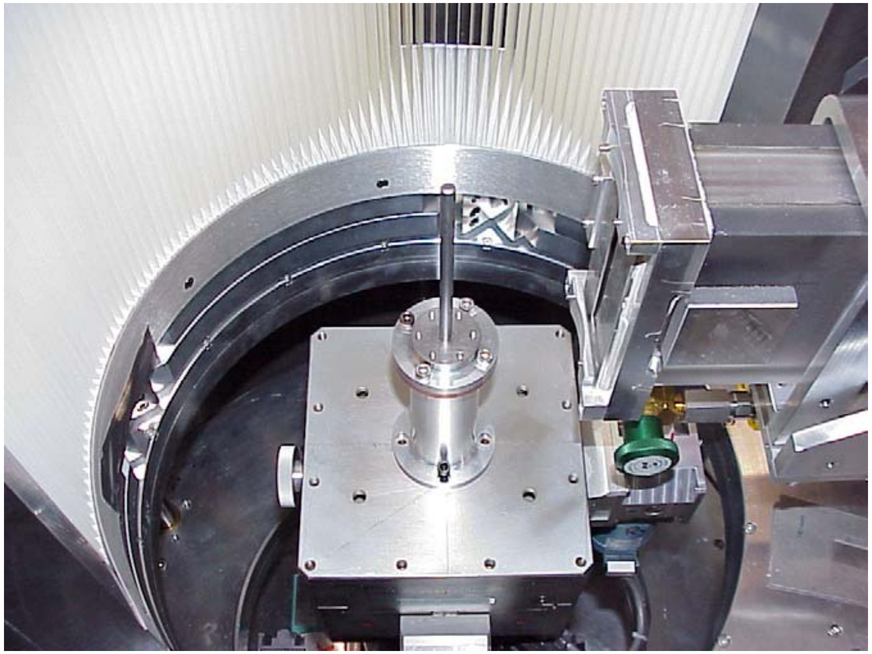






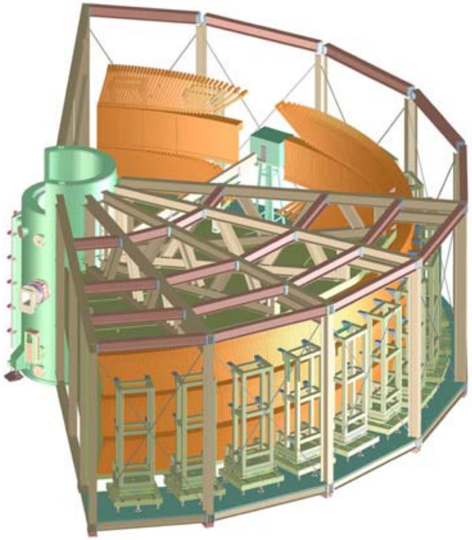
(4) The sample area

The sample stage accomodates a wide variety of sample environments.
A radial collimator reduces scattering from vacuum cans, radiation shields, etc.

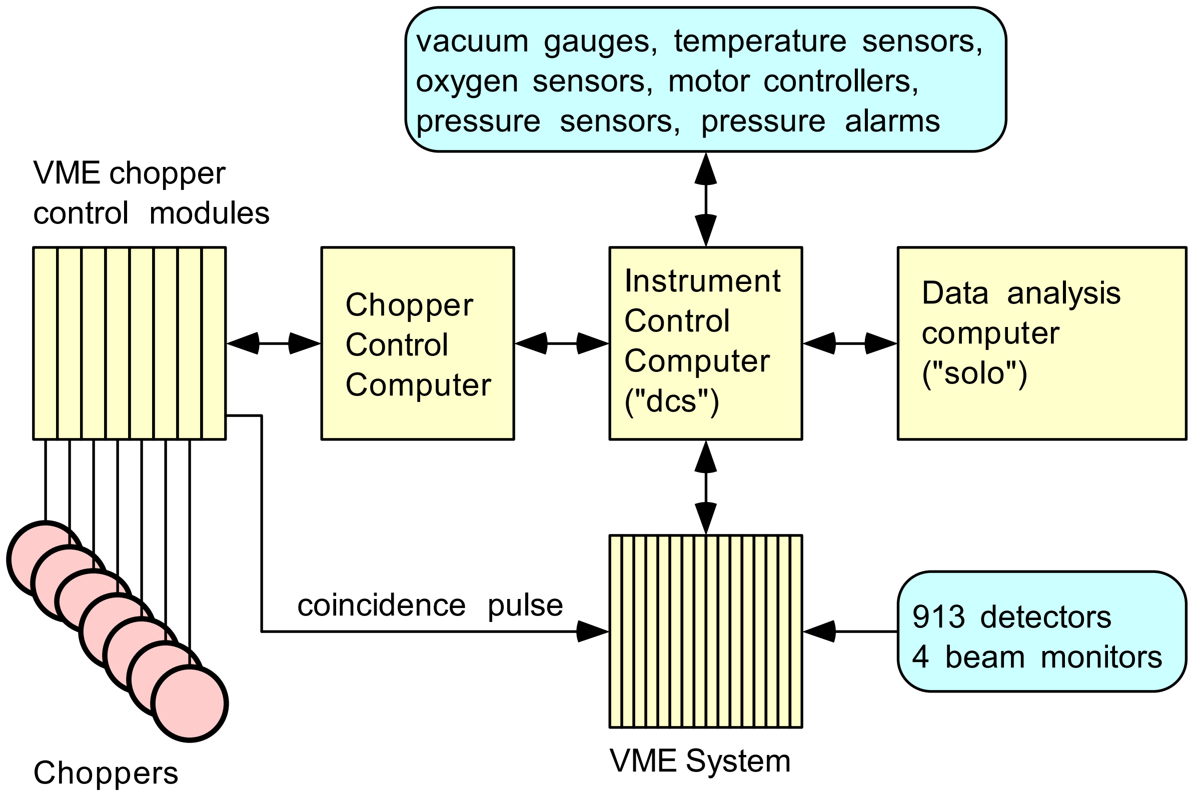


(5) The flight chamber and the detectors

The flight chamber is argon-filled to reduce scattering of neutrons traveling from the sample to the detectors.
There are 913 detectors in 3 banks.



Instrument control and data acquisition system



Trading intensity I(E) for resolution ΔE

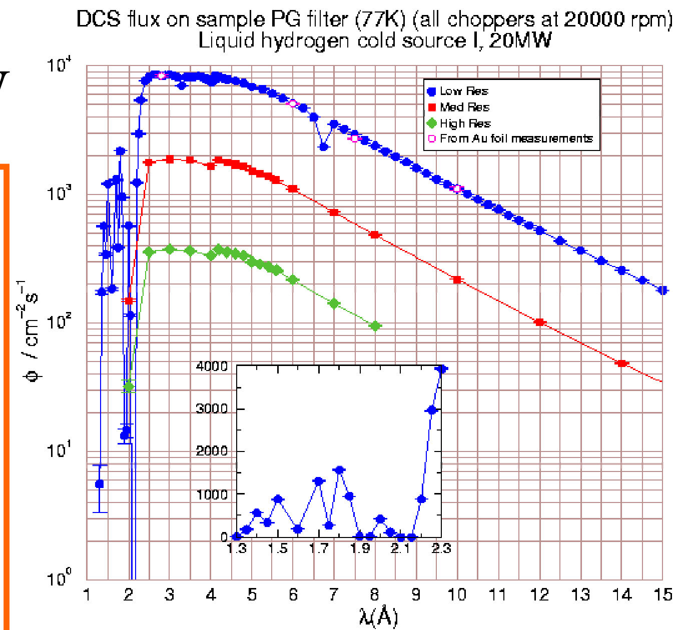
Quantities that can be varied:

- chopper period T, and "frame overlap ratio" $m=T_S/T$
- wavelength λ
- chopper slot widths W

(T_S is the period at the sample)

Q range $\propto 1/\lambda$

E range increases as m increases, but $I(E) \propto 1/m$

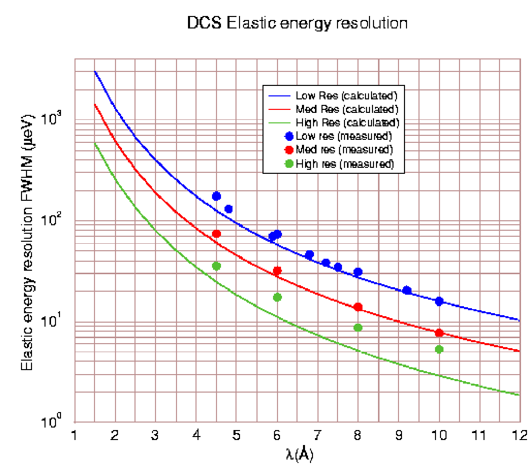


At fixed T and W:

I(E) peaks: 2.5-4.5A

At long λ, I(E) drops ~50% for every 2A.

ΔE varies as $\sim\lambda^{-3}$



At fixed λ, W:

$I(E) \propto T^2 / T_S$

$\Delta E \propto T$

At fixed λ, T:

$I(E) \sim \propto W^3$

$\Delta E \sim \propto W$